Semileptonic Decays of D Mesons in Three-Flavor Lattice QCD

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We present the first three-flavor lattice QCD calculations for $D \to \pi l \nu$ and $D \to K l \nu$ semileptonic decays. Simulations are carried out using ensembles of unquenched gauge fields generated by the MILC Collaboration. With an improved staggered action for light quarks, we are able to simulate at light quark masses down to 1/8 of the strange mass. Consequently, the systematic error from the chiral extrapolation is much smaller than in previous calculations with Wilson-type light quarks. Our results for the form factors at $q^2 = 0$ are $f_+^{D\to\pi}(0) = 0.64(3)(6)$ and $f_+^{D\to K}(0) = 0.73(3)(7)$, where the first error is statistical and the second is systematic, added in quadrature. Combining our results with experimental branching ratios, we obtain the Cabibbo-Kobayashi-Maskawa matrix elements $|V_{cd}| = 0.239(10)(24)(20)$ and $|V_{cs}| = 0.969(39)(94)(24)$, where the last errors are from experimental uncertainties.

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Semileptonic decays of heavy-light mesons are of great interest because they can be used to determine Cabibbo-Kobayashi-Maskawa (CKM) matrix elements such as $|V_{ub}|$, $|V_{cb}|$, $|V_{cd}|$, and $|V_{cs}|$. The accuracy of one of the most important, $|V_{ub}|$, is currently limited by large theoretical uncertainty [1]. Lattice QCD provides a systematically improvable method of calculating the relevant hadronic amplitudes, making the determination of $|V_{ub}|$ and other CKM matrix elements more reliable and precise.

Semileptonic D meson decays, such as $D \to K l \nu$ and $D \to \pi l \nu$, provide a good test of lattice calculations, because the corresponding CKM matrix elements $|V_{cs}|$ and $|V_{cd}|$ are known more accurately than $|V_{ub}|$ [1]. The decay rates and distributions are not yet very well known, but the CLEO-c experiment plans to measure them with an accuracy of a few per cent. Furthermore, measurements of leptonic and semileptonic $D_{(s)}$ decays can be combined so that the CKM matrix drops out, offering a direct and stringent check of lattice QCD.

Recently, dramatic progress has been achieved in lattice QCD, for a wide variety of hadronic quantities. Reference [2] showed agreement at the few percent level between three-flavor lattice QCD and experiment for f_π, f_K, mass splittings of quarkonia, and masses of heavy-light mesons. The main characteristics of these quantities are that they have at most one stable hadron in the initial and final states, and that the chiral extrapolation from simulated to physical light quark masses is under control. This class can be called "gold plated" [2], and many of the lattice calculations needed to test the Standard Model are in this class. The work reported here is part of a systematic effort to calculate the hadronic matrix elements needed for leptonic and semileptonic decays, and for neutral meson mixing [3,4].

In this Letter we report results for $D \to K l \nu$ and $D \to \pi l \nu$ semileptonic decay amplitudes. All previous lattice calculations of heavy-light semileptonic decays have been done in quenched ($n_f = 0$) QCD. In addition to quenching, they also suffered from large uncertainties from the chiral extrapolation and, in some cases, from large heavy-quark discretization effects. Here we bring all three uncertainties under good-to-excellent control. Indeed, this Letter presents the first calculation in unquenched three-flavor lattice QCD, where the effect of dynamical u, d, and s quarks is correctly included.

The relevant hadronic amplitude $\langle P|V^\mu|D\rangle$ ($P = \pi, K$) is conventionally parametrized by form factors f_+ and f_0 as

$$\langle P|V^\mu|D\rangle = f_+(q^2)(p_D + p_P - \Delta)^\mu + f_0(q^2)\Delta^\mu \quad (1)$$

where $q = p_D - p_P$, $\Delta^\mu = (m_D^2 - m_P^2)q^\mu/q^2$. The differential decay rate $d\Gamma/dq^2$ is proportional to $|V_{cx}|^2|f_+(q^2)|^2$, $x = d, s$. (A contribution from f_0 is proportional to the lepton mass squared.) We calculate f_+ and f_0 as a function of q^2 and determine the decay rate Γ and the CKM matrix $|V_{cx}|$ by integrating $|f_+(q^2)|^2$ over q^2. Preliminary results have been reported in Ref. [4,5].

Our calculations use ensembles of unquenched gauge fields generated by the MILC collaboration [6] with the "Asqtad" improved staggered quark action and the Symanzik-improved gluon action [7]. The results are obtained on the "coarse" ensembles with sea quark masses $am_l^{\rm sea} = 0.005$, 0.007, 0.01, 0.02, and 0.03. The gauge coupling is adjusted to keep the same lattice cutoff ($a^{-1} \approx$ 1.6 GeV) and volume [$L^3 \times T \approx (2.5\ {\rm fm})^3 \times 8.0$ fm]. Each ensemble has about 400–500 configurations. For more information on these ensembles, including autocorrelations, see Ref. [6].

For the light valence quarks, we adopt the same staggered action as for the dynamical quarks. The valence light (u, d) quark mass $m_l^{\rm val}$ is always set equal to $m_l^{\rm sea}$. The valence strange quark mass is $am_s^{\rm val} = 0.0415$, which is slightly larger than the physical value $am_s = 0.039$ (at this lattice spacing) determined from fixing the masses of the light pseudoscalars [6]. We have repeated the calculations with a strange quark mass slightly too small, and find a negligible difference. Since the computation of the staggered propagator is fast, we can simulate with m_l as low as $m_s/8$. Consequently we are able to reduce the systematic error from the chiral extrapolation ($m_l \to m_{ud}$) to $\approx 3\%$, as we show below. In contrast, previous calculations with Wilson-type light quarks simulated at $m_l \geq m_s/2$ and typically had $O(10\%)$ errors from this source alone [8].

For the valence charmed quark we use the clover action with the Fermilab interpretation [9]. The bare mass is fixed via the D_s kinetic mass [3]. The free parameters of both the action and the current are adjusted so that the leading heavy-quark discretization effects are $O(\alpha_s a\Lambda_{\rm QCD})$ and $O[(a\Lambda_{\rm QCD})^2]$, where $\Lambda_{\rm QCD}$ is a measure of the QCD scale.

The hadronic matrix element $\langle P|V^\mu|D\rangle$ is extracted from the three-point function in the D meson rest frame ($\boldsymbol{p}_D = 0$)

$$C_{3,\mu}^{D\to P}(t_x, t_y; \boldsymbol{p}) = \sum_{x,y} e^{i\boldsymbol{p}\cdot\boldsymbol{y}}\langle O_P(0)\hat{V}_\mu(y)O_D(x)\rangle, \quad (2)$$

where $\boldsymbol{p} = \boldsymbol{p}_P$, $\hat{V}_\mu = \bar{\psi}_c\gamma_\mu\psi_x$ ($x = d$, s) is the heavy-light vector current on the lattice, and O_D and O_P are interpolating operators for the initial and final states. The heavy-light bilinears $\hat{V}_\mu$ and O_D are formed from staggered light quarks and Wilson heavy quarks as in Ref. [10]. The three-point functions are computed for light meson momentum $\boldsymbol{p}$ up to $2\pi(1, 1, 1)/L$, using local sources and sinks. The sink time is fixed typically to $t_x = 20$. To increase the statistics, the calculations are carried out not only at the source time $t_0 = 0$ but also at $t_0 = 16$, 32, 48, (and t_x and t_y shifted accordingly). The results from four source times are averaged. Statistical errors are estimated by the jackknife method. To extract the transition amplitude $\langle P|V^\mu|D\rangle$ we also need meson two-point functions $C_2^M(t_x; \boldsymbol{p}) = \sum_{\boldsymbol{x}} e^{i\boldsymbol{p}\cdot\boldsymbol{x}}\langle O_M(0)O_M^\dagger(x)\rangle$, where $M = D$, π, K. They are computed in an analogous way. For the light meson ($M = \pi$, K) the two-point function couples to the Goldstone channel of staggered quarks.

A drawback of staggered quarks is that each field produces four quark species, called "tastes" to stress that the extra three are unphysical. There are three important consequences that should be mentioned. First, the number of tastes of sea quarks is reduced to two or one by taking the square root or fourth root of the four-taste fermion determinant. The validity of this procedure is not yet proven and warrants further study.

Second, the light meson two-point function contains a 16-fold replication of the desired hadrons. The heavy-light two-point function C_2^D does *not* suffer from such replication, because contributions of heavy quarks with momentum $p \sim O(\pi/a)$ are suppressed [10]. The same holds for three-point functions that include at least one Wilson quark, such as $C_{3,\mu}^{D\to P}$. To check these properties, we carried out a preparatory quenched calculation [4], finding reasonable agreement with those obtained previously with Wilson light quarks [8].

Finally, the three-point and two-point functions receive contributions from states that oscillate in time, in addition to the ground state and nonoscillating excited state contributions. For example, the three-point function's time dependence takes the form

$$C_{3,\mu}^{D\to P}(t_x, t_y) = A_0 e^{-E_P t_y} e^{-E_D(t_x - t_y)} + (-1)^{t_y} A_1 e^{-E' t_y} e^{-E_D(t_x - t_y)} + \cdots, \quad (3)$$

where $A_0 \propto \langle P|V^\mu|D\rangle$.

As usual, the desired hadronic amplitude is extracted from fitting the three-point and two-point functions. We employ two methods. In the first method, we form the ratio $R(t_y) \equiv C_{3,\mu}^{D\to P}(t_x, t_y)/[C_2^P(t_y)C_2^D(t_x - t_y)]$, and fit to a constant in t_y. The oscillating state contributions are partly canceled in the ratio, and further reduced by taking the average, $\bar{R}(t_y) = [R(t_y) + R(t_y + 1)]/2$. A plateau is then found for t_y around $t_x/2$. In the second method, we first fit $C_{3,\mu}^{D\to P}$ and $C_2^{P,D}$ separately, using a multiexponential form similar to Eq. (3), and then obtain $\langle P|V^\mu|D\rangle$ from the fit results. The results from the two methods always agree within statistical errors. The difference between two results is less than 3% for the lower two momenta, and as large as 3% for the higher two momenta. We choose the first method for central values and take 3% as the systematic error from the fitting.

The lattice heavy-light vector current must be multiplied by a renormalization factor $Z_{V_\mu}^{cx}$. We follow the method in Ref. [8], writing $Z_{V_\mu}^{cx} = \rho_{V_\mu}(Z_V^{cc} Z_V^{xx})^{1/2}$. The flavor-conserving renormalization factors Z_V^{cc} and Z_V^{xx} are computed nonperturbatively from standard charge normalization conditions. The remaining factor ρ_{V_μ} is expected to be close to unity because most of the radiative corrections are canceled in the ratio [11]. A one-loop calculation gives [12] $\rho_{V_4} \approx 1.01$ and $\rho_{V_i} \approx 0.99$ which we use in the analysis below. This perturbative calculation is preliminary, but it has been subjected to several nontrivial tests.

Rather than calculating the conventional form factors f_0 and f_+ directly, we first extract the form factors $f_\parallel$ and $f_\perp$, as in Ref. [8], defined through

$$\langle P|V^\mu|D\rangle = \sqrt{2m_D}[v^\mu f_\parallel(E) + p_\perp^\mu f_\perp(E)], \qquad (4)$$

where $v = p_D/m_D$, $p_\perp = p_P - Ev$ and $E = v \cdot p_P$ is the energy of the light meson. $f_\parallel$ and $f_\perp$ are more natural quantities in the heavy-quark effective theory, and chiral expansions are given for them as a function of E [13,14]. We therefore carry out the chiral extrapolation in m_l for $f_\parallel$ and $f_\perp$ at fixed E, and then convert to f_0 and f_+.

To perform the chiral extrapolation at fixed E, we interpolate and extrapolate the results for $f_\parallel$ and $f_\perp$ to common values of E. To this end, we fit $f_\parallel$ and $f_\perp$ simultaneously using the parametrization of Becirevic and Kaidalov (BK) [15],

$$f_+(q^2) = \frac{F}{(1-\tilde{q}^2)(1-\alpha\tilde{q}^2)}, \quad f_0(q^2) = \frac{F}{1-\tilde{q}^2/\beta}, \qquad (5)$$

where $\tilde{q}^2 = q^2/m_{D_x^*}^2$, and $F = f_+(0)$, α and β are fit parameters, and f_+, f_0, and q^2 are converted to $f_\parallel$, $f_\perp$, and E before the fits. An advantage of the BK form is that it contains a pole in $f_+(q^2)$ at $q^2 = m_{D_x^*}^2$, where $m_{D_x^*}$ is the lattice mass of the charmed vector meson with daughter quark x. The BK fit for $f_\perp$ is shown in Fig. 1, using data for all available momenta $\boldsymbol{p}$. Excluding the data for the highest momentum $2\pi(1, 1, 1)/L$ gives indistinguishable results.

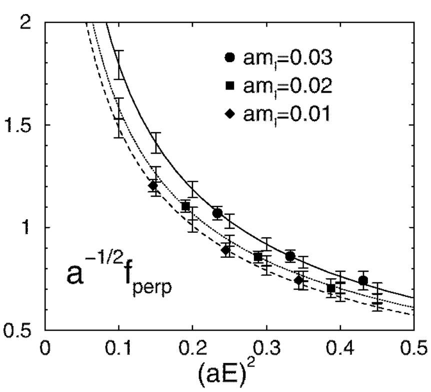

FIG. 1. $a^{-1/2}f_\perp$ as a function of $(aE)^2$ for the $D \to \pi$ decay. Symbols are raw data and lines are fitting curves with the parametrization of Eq. (5). Results at $m_l = 0.03$, 0.02, and 0.01 are shown.

We perform the chiral extrapolation using recently obtained expressions [14] for heavy-to-light form factors in staggered chiral perturbation theory (SχPT) [16]. As in continuum χPT [13], the formulae contain the chiral coupling f and heavy-to-light meson coupling g. We take $f = 130$ MeV and $g = 0.59$, but changing these constants by 10% has negligible effect. The SχPT formulae contain six additional parameters (4 splittings and two taste-violating hairpins) to parameterize lattice discretization effects. The new parameters are fixed from the analysis of light pseudoscalars [6]. The fit form we adopt ("SχPT + linear") is

$$f_{\perp,\parallel}(E) = A[1 + \delta f_{\perp,\parallel}(E)] + Bm_l, \qquad (6)$$

where A, B are fit parameters, and $\delta f_{\perp,\parallel}$ is the SχPT correction. To estimate the systematic error here, we try a simple linear fit and a "SχPT + quadratic" fit with a term Cm_l^2 added to Eq. (6). A comparison of the three fits is shown in Fig. 2. For the $D \to \pi(K)$ decay the linear fit gives 3% (2%) larger results at $m_l = m_{ud}$. The results from the SχPT + quadratic fit typically lie between the results from the other two fits, with larger errors. We therefore take 3% (2%) as the systematic error from the chiral extrapolation for the $D \to \pi(K)$ decay.

We now convert the results for $f_\perp$ and $f_\parallel$ at $m_l = m_{ud}$, to f_+ and f_0. To extend f_+ and f_0 to functions of q^2, we again fit to the form Eq. (5). The results are shown in Fig. 3, with statistical errors only. We then obtain the decay rates $\Gamma/|V_{cx}|^2$ by integrating (phasespace) $\times$ $|f_+(q^2)|^2$ over q^2. Finally, we determine the CKM matrix elements $|V_{cd}|$ and $|V_{cs}|$ using experimental lifetimes and branching ratios [1]. These main results are summarized in Table I.

The results presented above rely on the q^2 dependence of BK parametrization, Eq. (5). To estimate the associated systematic error, we make an alternative analysis without it. We perform a two-dimensional fit in (m_l, E) to the raw data employing a polynomial form plus the SχPT correction $\delta f_{\parallel,\perp}$. The result from this fit agrees with the one from

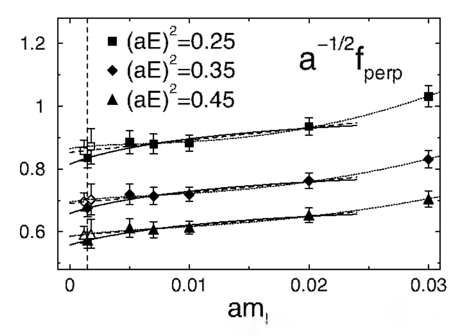

FIG. 2. m_l dependence and chiral fits for $a^{-1/2}f_\perp^{D\to\pi}$ for several values of $(aE)^2$. The SχPT + linear fit (solid line), SχPT + quadratic fit (dotted line) and linear fit (dashed line).

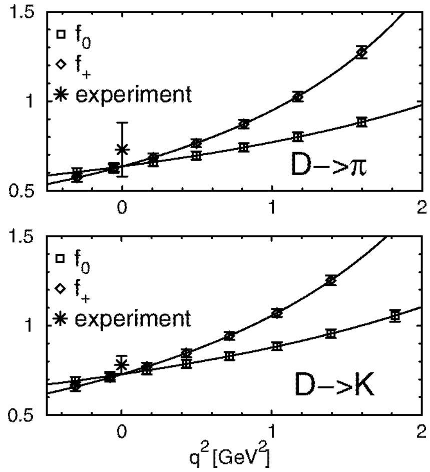

FIG. 3. $D \to \pi$ and $D \to K$ form factors. The experimental values are taken from Ref. [19].

the fit with Eq. (6) within statistical errors. The deviation between the two fits is negligible at $q^2 \sim q^2_{\rm max}$ and about 1σ at $q^2 \sim 0$ for $f_{\perp,\parallel}$, giving a 2% difference for the CKM matrix elements.

With only one lattice spacing, the systematic error from discretization effects can be estimated only by power counting. The leading discretization errors from the Asqtad action are $O[\alpha_s(a\Lambda_{\rm QCD})^2] \approx 2\%$ (after removal of taste-violating effects with SχPT), taking $\Lambda_{\rm QCD} = 400$ MeV and $\alpha_s = 0.25$. In addition, there is a momentum-dependent error from the final state. The BK parameters are determined by the lower momentum data;, in particular, the fits are insensitive to the highest momentum $2\pi(1, 1, 1)/L$. Therefore we estimate this effect to be $O[\alpha_s(a\boldsymbol{p})^2] \approx 5\%$, taking the second-highest momentum $\boldsymbol{p} = 2\pi(1, 1, 0)/L$. The heavy-quark effective theory (HQET) of cutoff effects [17,18] can be used to estimate the discretization error from the heavy charmed quark. In this way, we estimate the discretization error to be 4–7%, depending on the value chosen for $\Lambda_{\rm QCD}$ (in the HQET context). This is consistent with the lattice spacing dependence seen in Ref. [8]. In future work we expect to reduce and understand better this uncertainty, so we shall adopt the maximum, 7%, here.

A summary of the systematic errors for the form factors $f_{+,0}$ or the CKM matrix elements $|V_{cx}|$ is as follows. The error from time fits is 3%; from chiral fits, 3% (2%) for $D \to \pi(K)$ decay; from BK parametrization, 2%. The 1-loop correction to ρ_{V_μ} is only 1%, so 2-loop uncertainty is assumed to be negligible. The uncertainty for a^{-1} is about 1.2% [6]; this leads to a 1% error for $|V_{cx}|$ (but not for the dimensionless form factors), from integrating over q^2 to get $\Gamma/|V_{cx}|^2$. Finally, we quote discretization uncertainties of 2%, 5%, and 7%, from light quarks, the final state energy, and the charmed quark, respectively. Adding all the systematic errors in quadrature, we find the total to be $[3\% + 3\%(2\%) + 2\% + 1\% + 2\% + 5\% + 7\%] = 10\%$.

TABLE I. Fit parameters in Eq. (5), decay rates, and CKM matrix elements. The first errors are statistical; the second systematic; the third experimental.

P	F	α	β	$\Gamma/\lvert V_{cx}\rvert^2[\mathrm{ps}^{-1}]$	$\lvert V_{cx}\rvert$
π	0.64(3)	0.44(4)	1.41(6)	0.154(12)(31)	0.239(10)(24)(20)
K	0.73(3)	0.50(4)	1.31(7)	0.093(07)(18)	0.969(39)(94)(24)

Incorporating the systematic uncertainties, we obtain

$$f_+^{D\to\pi}(0) = 0.64(3)(6), \tag{7}$$

$$f_+^{D\to K}(0) = 0.73(3)(7), \tag{8}$$

and the ratio $f_+^{D\to\pi}(0)/f_+^{D\to K}(0) = 0.87(3)(9)$. Our results for the CKM matrix elements (Table I) are consistent with Particle Data Group averages $|V_{cd}| = 0.224(12)$ and $|V_{cs}| = 0.996(13)$ [1]; also with $|V_{cs}| = 0.9745(8)$ from CKM unitarity. If we instead use these CKM values as inputs, we obtain, for the total decay rates,

$$\Gamma(D^0 \to \pi^- l^+ \nu) = (7.7 \pm 0.6 \pm 1.5 \pm 0.8) \times 10^{-3}\,\mathrm{ps}^{-1},$$
$$\Gamma(D^0 \to K^- l^+ \nu) = (9.2 \pm 0.7 \pm 1.8 \pm 0.2) \times 10^{-2}\,\mathrm{ps}^{-1},$$
$$\frac{\Gamma(D^0 \to \pi^- l^+ \nu)}{\Gamma(D^0 \to K^- l^+ \nu)} = 0.084 \pm 0.007 \pm 0.017 \pm 0.009, \tag{9}$$

where the first errors are statistical, the second systematic, and the third from uncertainties in the CKM matrix elements. We do not assume any cancellation of errors in the ratios, although some may be expected. Our results agree with recent experimental results, $f_+^{D\to\pi}(0) = 0.73(15)$, $f_+^{D\to K}(0) = 0.78(5)$ [19], $f_+^{D\to\pi}(0)/f_+^{D\to K}(0) = 0.86(9)$, and $\Gamma(D^0 \to \pi^- e^+ \nu_e)/\Gamma(D^0 \to K^- e^+ \nu_e) = 0.082 \pm 0.008$ [20].

This Letter presents the first three-flavor lattice calculations for semileptonic D decays. With an improved staggered light quark, we have successfully reduced the two dominant uncertainties of previous works, i.e., the effect of the quenched approximation and the error from chiral extrapolation. Our results for the form factors, decay rates and CKM matrix, given in Table I and Eq. (9) are in agreement with experimental results. The total size of systematic uncertainty is 10%, which is dominated by the discretization errors. To reduce this error, calculations at finer lattice spacings and with more highly improved heavy-quark actions are necessary; these are underway. Finally, unquenched calculations of B decays such as $B \to \pi l \nu$ and $B \to D l \nu$ are in progress, and will be presented in a separate paper.

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